

Sample File:

DSSTox Log File:

EPA Water Disinfection By-Products with Carcinogenicity Estimates (DBPCAN)

(last updated 19 October 03)

Description: Information in this file documents the DBPCAN SDF file creation, review, and update process, provides summary information on database content, and lists currently unavailable CAS information for known structures. The first section summarizes the process used for creating the initial DSSTox SDF files and the quality assurance checks and procedures employed. A table providing field and data counts offers summary overview of the database content and chemical composition. The Log table will document any future modifications and revisions to the database content or format. For the most current version of this Log File and a record of any new modifications, or to report errors in this file, a user should consult the central DSSTox website: <http://www.epa.gov/nheerl/dsstox/>

QA and Development Notes:

Data included in DBPCAN underwent a series of quality review checks prior to publication of initial launch version. The original database was obtained from reference materials associated with the Main Citation and from communication with the Source and main authors of that study. We thank Yin-tak Woo for providing the most current data tables in electronic form. Chemical structures were initially obtained by conversion of SMILES codes provided in the original database using CambridgeSoft's ChemOffice 2002 ChemDraw (ver 7.0 for Windows) for MS Excel. Structures were further verified against drawn structures and names in Source-provided materials. The ChemFinder website (<http://chemfinder.cambridgesoft.com/>) was used for checking CAS-to-structures and for retrieving "AnalogCAS" numbers for analogs of the predicted chemical. CambridgeSoft ChemFinder (ver 7.0 for Windows) was also used for automatic generation of SMILES codes from structures and both ChemFinder and ACD ChemFolder (ver 6.0 for Windows) were employed for "Structure-to-Name" or "Name-to-Structure" features. Original SMILES codes provided by the Source were converted to ChemFinder-generated SMILES when the former could not be converted to a Structure and verified within the ChemFinder application.

ChemName, SMILES, CAS and Structure field contents were checked by cross-referencing wherever possible. Since this database contained no "salt" or "complex" forms, no "defined organic parent" (DOP) SDF file was created containing simplified parent structures.

Field and Data Counts in DSSTox SDF file: Refer to DBPCAN_FieldDefFile for definitions and explanations of all terms.

DSSTox SDF	Standard Chemical Fields	Source-specific fields	Chemical records total	Defined organic	Inorganic	Organo-metallic	Mixture or unknown	Parent	Salt or Salt complex	Complex
DBPCAN_v1a	11	9	209*	204	5	0	0	209	0	0

*Three pairs of replicate 2D structures exists in the database (cis/trans isomer pairs).

Log of SDF Modifications and Version/revision updates:

Date	DSSTox SDF File Name	Modifications from previous version	Additional Notes
12Sep03	DBPCAN_v1a_209_12Sep03.sdf	Initial launch publication; no previous published versions.	DBPCAN is considered a "static" historical database meaning that further expansion of the database to include additional data is unlikely. Future updates will correct reported errors provided by users or incorporate DSSTox format changes.

Wanted!! CAS Information

The **Unknown** CAS entries below are primarily an indication of the unstudied nature of many of the disinfection by-product entries in the DBPCAN database. However, if a user has information pertaining to any **Unknown** CAS in the below listing, please report this using a [DSSTox Error Report Form](#) that can be accessed from any DSSTox SDF Download Page, and be sure to indicate all relevant information (full DSSTox SDF file name, DSSTox_ID, ChemName, nature of missing information, source of correct information, etc.). Thank you!

ChemName	Structure or SMILES	CAS	SDF	Date of Request
1,2-Bis(1-methylethenyl)-benzene	<chem>C1=C(C(C)=C)C(C(C)=C)=CC=C1</chem>	Unknown	DBPCAN	12Sep03
Bromoamine	<chem>NBr</chem>	Unknown	DBPCAN	12Sep03
Bromochloromethyl acetate	<chem>BrC(OC(C)=O)Cl</chem>	Unknown	DBPCAN	12Sep03
3-Bromo-4-(dibromomethyl)-5-hydroxy-2(5H)-furanone	<chem>OC1OC(C(Br)C1C(Br)Br)=O</chem>	Unknown	DBPCAN	12Sep03
1-Bromo-1,1-dichloropropanone	<chem>O=C(C)C(Cl)(Br)Cl</chem>	Unknown	DBPCAN	12Sep03
3-Bromopropylchloromethyl ether	<chem>BrCCCCOCCl</chem>	Unknown	DBPCAN	12Sep03
tert-Butyl-cis-butenedioic acid	<chem>O=C(O)C=C(C(C)(C)(C))C(O)=O</chem>	Unknown	DBPCAN	12Sep03
3-Chloro-4-(bromochloromethyl)-5-hydroxy-2(5H)-furanone	<chem>O=C1OC(O)C(C(Br)Cl)=C1Cl</chem>	Unknown	DBPCAN	12Sep03

... Table truncated for SampleFile use.